Deuterium chemistry in protoplanetary disks

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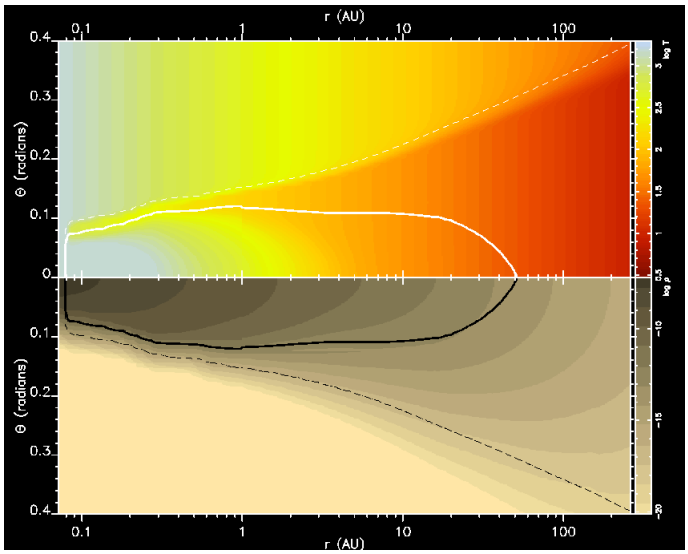
Introduction

Observations of deuterated molecules give important information about the temperature conditions present at the time of their formation. In protoplanetary disks they may provide a means of tracing the evolution of planets. In cold dark clouds molecules are observed to have a high deuterium fractionation as a consequence of formation in cold conditions. In hot cores, the high deuteration rates seen are attributed to the evaporation of icy grain mantles accreted during an earlier molecular cloud phase. Recently the first deuterated molecules have been detected in protostellar disks (HDO, DCN, Kessler et al. 2002), DCO^+ (van Dishoeck et al. 2003) and H_2D^+ (Ceccarelli et al. 2004). Here we present the results from a deuterium chemical model of a protostellar disk and compare our results with the available observations. Chemical modeling combined with observations provides important information about disks as they evolve and form planets.



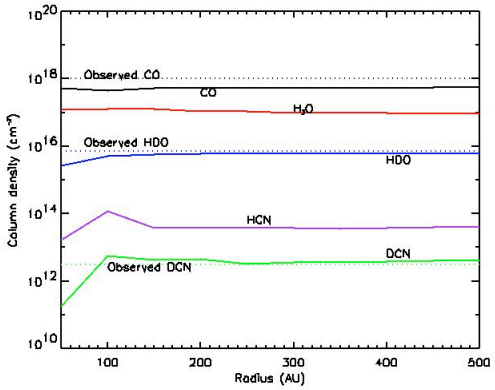
The disk structure as calculated by Bryden et al. (2004) for a model with mass accretion rate = 10^{-8} $M_\odot$ and Σ_0 = 1000gcm^{-2} at 1AU. The top panel shows temperature in the disk and the bottom panel the density structure. The solid dark line shows the surface of the disk based on the vertical depth of its own infrared radiation, while the dotted line plots the optical surface to radial, visible stellar radiation. Model disk mass = 0.06 $M_\odot$

Chemical model:

- Ratefile from UMIST database RATE97 (Millar et al. 1997).
- Deuterium chemistry based on Willacy & Millar (1998)
- Input abundances from output of molecular cloud model at 1Myrs
- Includes gas/grain interactions - freezeout, thermal desorption, cosmic ray heating, photodesorption and grain surface reactions
- Includes photoprocessing due to both stellar and interstellar UV field (stellar UV field = 500x ISRF - Bergin et al. 2003).

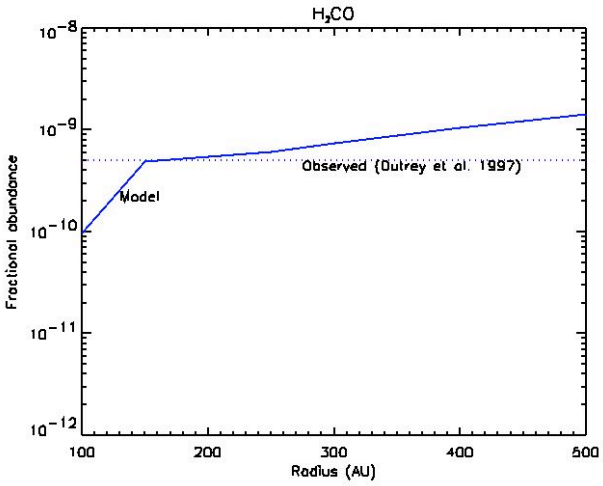
Results - Column densities

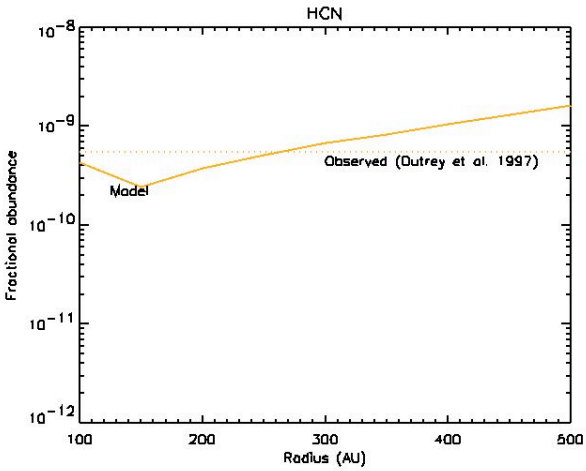
We compare results to available observations - one problem is that there is no complete inventory of deuterated and non-deuterated molecules in a single source. We therefore use observations of three different T-Tauri stars, LkCa15, DM Tau and TW Hya - stars with similar disk masses, mass accretion rates and ages to that assumed in the models. Results are shown for model time of 1 Myrs



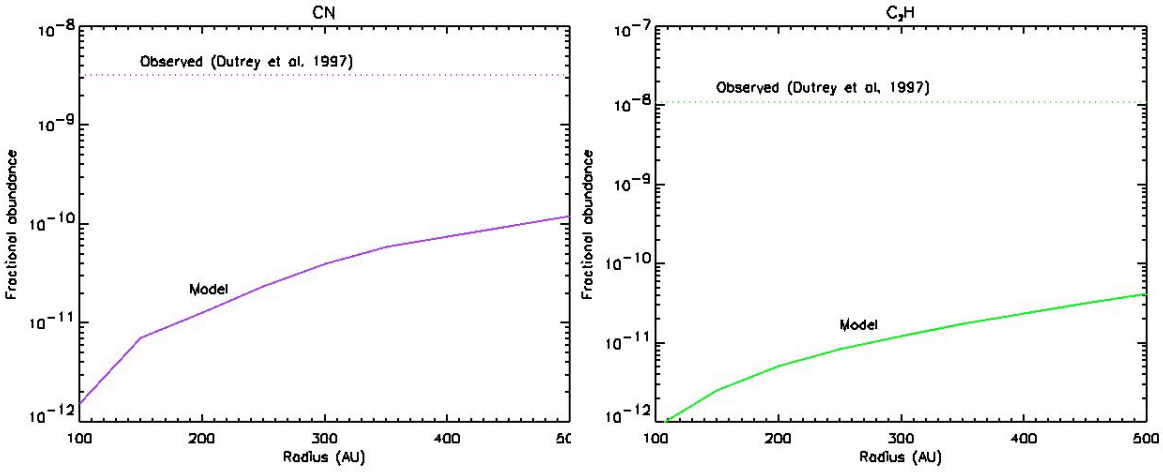
- Column densities calculated in this model (solid lines) and observed in LkCa15 (dashed lines) (Kessler 2003).
- Calculated column densities of these molecules show little variation with R
- Good agreement with observations of LkCa15 in outer disk.

Results - Fractional abundances



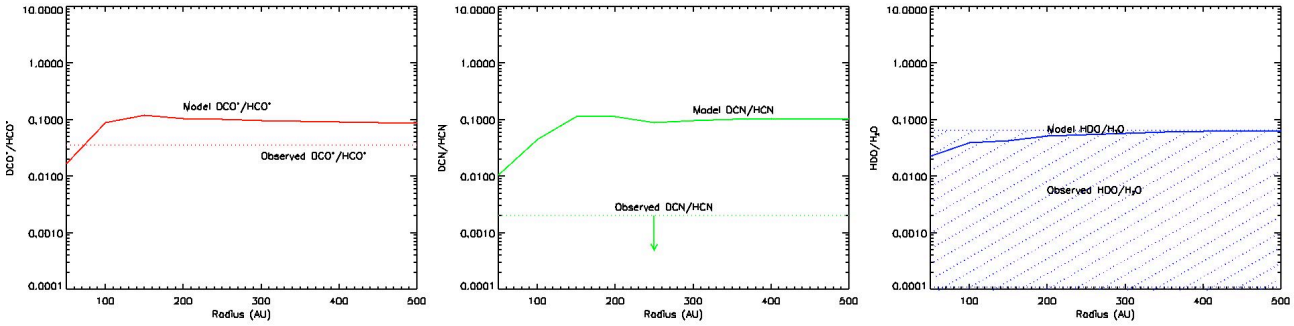


Good agreement with fractional abundances for most molecules observed by Dutrey et al. (1997) in DM Tau



However our models predict too little for the abundances of photodissociation products such as CN and C_2H (a factor of > 100 underabundant)

Results - D/H ratios



- Observational data from Kessler (2003) (HCN and HDO - LkCa15) and van Dishoeck et al (2003) (DCO^+ - TW Hya)
- N(DCO^+) factor of 10 lower than observed (although D/H ratios agree with observations)
- DCN/HCN ratio too high - N(DCN) agrees with observations, N(HCN) too low.
- Good agreement for HDO deuteration ratios

Conclusion - The good agreement between the models and the observations suggests that disk chemical models will be of use in interpreting the observed D/H ratios.

References

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Acknowledgements

This research was carried out at the Jet Propulsion Laboratory, California Institute of Technology under contract with the National Aeronautics and Space Administration, and was supported by grants from the NASA Origins and TPF Foundation Science programs